

EXAFS study in epitaxial SrTiO₃ thin films on Silicon

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Introduction: SrTiO₃/Si(001) has a wide range of potential applications, such as a dielectric gate in MOSFET devices [1], where the film thickness plays a very important role on the electrical properties. The aim of this study is to investigate the local structure in epitaxial STO/Si(001) before and after its critical thickness.

Methods and Materials: Epitaxial SrTiO₃ on Si(001) was studied with extended x-ray absorption fine structure (EXAFS). The strontium titanate thin films were previously grown on Si(001) by molecular beam epitaxy (MBE) for thickness of 200, 60 and 40 Å. The data was recorded in the fluorescence mode for the Ti K-edge with the synchrotron electric field either parallel or perpendicular to the surface plane.

Results: The gradual change on the Ti-O peak for the in-plane data (Figure 1) is in accordance to an epitaxial mode of growth where the unit cell is elastically strained. However for the perpendicular direction (out-of-plane) the amplitude of the Ti-O peak for thinner films is dramatically reduced. This, in combination with the increase and shift to lower energies of the pre-edge feature [2] (Figure 2), indicates a loss in oxygen coordination. The decrease of the oxygen coordination cannot solely account for the reduction of the Ti-O peak, so disorder also plays a role. This is as well in accordance to the broadening on the peak right after the main jump [2], also shown in Figure 2.

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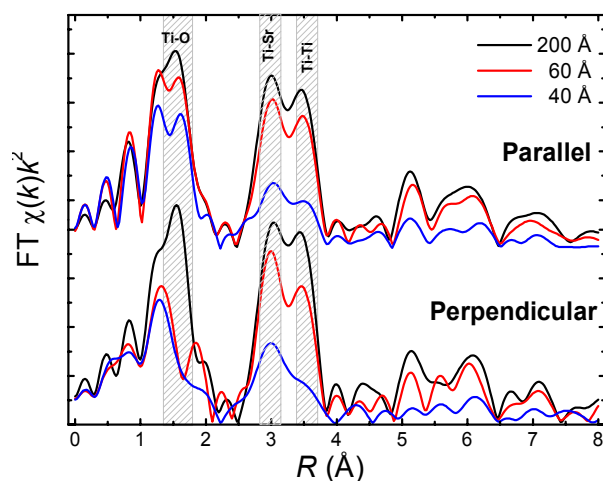


Figure 1. Fourier transform of the EXAFS data for each polarization for different thickness considered (200, 60 and 40 Å).

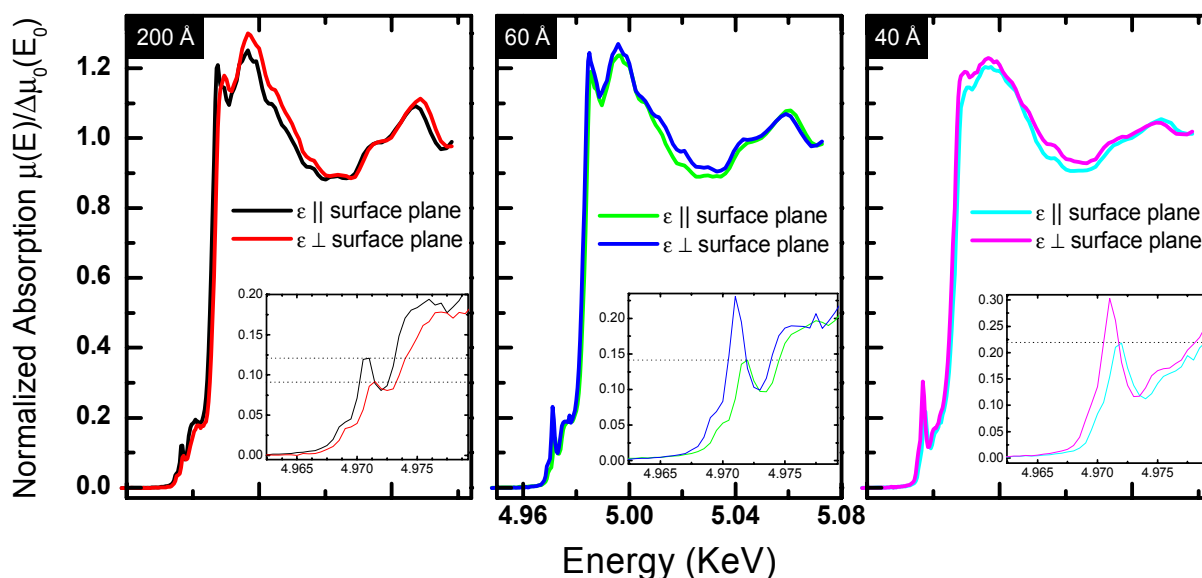


Figure 2. Ti K-edge XANES spectra collected for STO/Si(001) samples for various thickness for both parallel and perpendicular polarizations.